

Spin Correlation Effects In a One Dimensional Electron Gas

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Abstract

The Singwi, Sjölander, Tosi, Land (SSTL) approach is generalized to study the spin-correlation effects in a one dimensional electron gas. It is shown that the SSTL approach is capable of generating results comparable to the more widely used STLS approach.

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1 Introduction

The Singwi, Tosi, Land and Sjölander (STLS) approach[1] is a powerful theoretical tool in going beyond the random phase approximation (RPA) in studying the short range correlation effects of an interacting electron gas. It was originally developed for the three dimensional (3D) electron gas. In the STLS approach the short range correlation effects are described by the local field correction $G(q)$ for the density response function.

The STLS approach is later applied to the two dimensional[2]–[4] and the one dimensional electron gas (1D)[5]–[7] with long range Coulomb or short range interactions.

The Lobo, Singwi and Tosi (LST) approach[8] was originally developed to calculate spin correlation effects in the interacting 3D electron gas. Although the calculated spin susceptibility is not in agreement with experiment, LST approach is applied to the two dimensional[9]–[11] and one dimensional electron gas[12],[13] problems.

In this paper, we study the validity of yet another attempt to go beyond RPA, the Singwi, Sjölander, Tosi and Land (SSTL) approach[14] which was originally developed for a 3D electron gas. It is proposed as an improvement over the STLS approach to better take into account the compressibility rule. For a review of the STLS, SSTL and LST approaches please see reference[15]. It is curious that though it is not very widely used, the SSTL approach is not investigated before for a low dimensional electron gas problem. It is therefore of interest to study the SSTL approach, to investigate its range of validity and to compare its results with the very widely used STLS approach. This is done in our earlier work for density correlations in a 1D electron gas[16].

In the present paper, we generalize the SSTL approach to study the spin correlation effects in a one dimensional interacting electron gas. The organization of the paper is as follows: In section II we present the SSTL approach. The results for the structural properties are given in section III. A discussion of our results and the performance of the SSTL approach is presented in section IV.

2 Formalism

The ground state of the electron gas at high density is paramagnetic. In a paramagnetic system the magnetic moments of the constituents are randomly distributed and their magnetic moment is averaged to zero. If we apply a weak external magnetic field to such a system, it will develop a paramagnetic spin moment. The response of the system to the field can be studied via its wave vector and frequency dependent paramagnetic susceptibility function. In noninteracting electron system, the Pauli paramagnetic susceptibility term is pronounced instead of the paramagnetic susceptibility term. On the other hand, in an interacting electron system we have short range Coulomb and exchange effects. Then, the Pauli value must be improved. In this study, we investigate these effects within the self-consistent calculation approximation (SSTL) as in the case of density–density correlations. Furthermore, it is assumed that our system is a Fermi liquid and the electrons are embedded in a uniform positive background so that the system is neutral.

In the self-consistent calculation approximation the wave vector and frequency dependent density and spin–density response functions, $\chi^d(q, \omega)$ and $\chi^s(q, \omega)$ respectively, are

$$\chi^d(q, \omega) = \frac{\chi_0(q, \omega)}{1 - \psi^s(q)\chi_0(q, \omega)}, \quad (1)$$

and

$$\chi^s(q, \omega) = -g^2 \mu_B^2 \frac{\chi_0(q, \omega)}{1 - \psi^a(q)\chi_0(q, \omega)}, \quad (2)$$

where $\chi_0(q, \omega)$ is the free electron polarizability, ψ^s (ψ^a) is the spin symmetric (spin anti-symmetric) potential, g is the Landé factor and μ_B is the Bohr magneton.

The system responds to the applied magnetic field through the free particle susceptibility modified by a local field correction. The static structure factor $S(q)$ and the magnetic static structure factor $\tilde{S}(q)$ are related to the dynamic response functions by the fluctuation-dissipation theorem as follows:

$$S(q) = \frac{1}{\pi n} \int_0^\infty d\omega \operatorname{Im} \{ \chi^d(q, \omega) \}, \quad (3)$$

and

$$\tilde{S}(q) = \frac{1}{\pi n g^2 \mu_B^2} \int_0^\infty d\omega \operatorname{Im} \{ \chi^s(q, \omega) \}. \quad (4)$$

In the mean field approximation, the effective potentials $\psi^s(q)$ and $\psi^a(q)$ are defined as

$$\psi^s(q) = V(q)[1 - G(q)], \quad \psi^a(q) = V(q)I(q), \quad (5)$$

where $V(q)$ is the one dimensional Fourier transform of the Coulomb potential, $G(q)$ and $I(q)$ are the static local field correction arising from the short range Coulomb correlation and exchange-correlation effects for the density and spin-density responses, respectively. In the SSTL approximation they are given in one dimension by

$$G(q) = -\frac{1}{n} \int \frac{dq'}{2\pi} \frac{q'}{q} \frac{V(q')}{V(q)} \frac{1}{\varepsilon(q)} [S(q - q') - 1], \quad (6)$$

and

$$I(q) = \frac{1}{n} \int \frac{dq'}{(2\pi)} \frac{q'}{q} \frac{V(q')}{V(q)} \frac{1}{\varepsilon(q)} [\tilde{S}(q - q') - 1], \quad (7)$$

where n is the one dimensional electron gas density. The Fermi wave vector k_F is related to the linear (1D) electron density as $n = 2g_\nu k_F / \pi$. The g_ν is the valley degeneracy and in this work we assume $g_\nu = 1$, which is the case for the quantum wire structures $GaAl/Al_xGa_{1-x}As$. In one dimension, the dimensionless density parameter is defined as $r_s = \pi / 4k_F a_B^*$, where $a_B^* = \varepsilon_0 / e^2 m^*$ is the effective Bohr radius with background dielectric function ε_0 and effective electron mass m^* . The $\varepsilon(q)$ is the static dielectric function which is given in terms of the density response function $\chi^d(q)$ as

$$\frac{1}{\varepsilon(q)} = 1 + V(q)\chi^d(q). \quad (8)$$

In the STLS approximation, the potential under the integral sign in Eq. (6) and in Eq. (7) is not screened by $\varepsilon(q)$.

The random phase approximation (RPA) describes the dielectric properties of the electron gas very successfully at high electron densities. In RPA the short range correlations are assumed to be absent, i.e, the local field correction $G(q) = 0$. As the density of the system is lowered, the exchange and the correlation effects become important. The Hubbard approach (HA) was developed to improve the RPA by introducing a local field correction taking into account the exchange hole around the electron. In HA, the local field correction for spin correlations, $I_H(q)$, is given by

$$I_H(q) = -\frac{1}{2} \frac{V \left(\sqrt{q^2 + k_F^2} \right)}{V(q)}. \quad (9)$$

The spin symmetric and spin antisymmetric pair correlation functions are related to the static structure factor and the magnetic structure factor by a Fourier transform in any dimension respectively. In one dimension

$$g(r) = 1 + \frac{1}{2} \int_0^\infty dq \cos(qr) [S(q) - 1], \quad (10)$$

and

$$\tilde{g}(r) = \frac{1}{2} \int_0^\infty dq \cos(qr) [\tilde{S} - 1]. \quad (11)$$

These can be written in terms of parallel spin pair correlation function, $g_{\uparrow\uparrow}(r)$, and antiparallel spin pair correlation function $g_{\uparrow\downarrow}(r)$ as

$$g(r) = \frac{1}{2} [g_{\uparrow\uparrow}(r) + g_{\uparrow\downarrow}(r)], \quad \tilde{g}(r) = \frac{1}{2} [g_{\uparrow\uparrow}(r) - g_{\uparrow\downarrow}(r)]. \quad (12)$$

The spin dependent potentials may be obtained by combining the $\psi^s(q)$ and $\psi^a(q)$ as

$$\psi_{\uparrow\uparrow}(q) = \psi^s(q) + \psi^a(q), \quad \psi_{\uparrow\downarrow}(q) = \psi^s(q) - \psi^a(q). \quad (13)$$

The static density and spin-density susceptibilities in the self consistent calculation approximation may be obtained easily from Eq. (1) and (2) as

$$\chi^d(q) = \frac{\rho(\varepsilon_F)k_F}{q} \frac{\ln \left| \frac{q - 2k_F}{q + 2k_F} \right|}{1 - \frac{16r_s k_F}{\pi^2 q} F(q) [1 - G(q)] \ln \left| \frac{q - 2k_F}{q + 2k_F} \right|}, \quad (14)$$

and

$$\chi^s(q) = \frac{g^2 \mu_B^2 \rho(\varepsilon_F) k_F}{q} \frac{\ln \left| \frac{q + 2k_F}{q - 2k_F} \right|}{1 + \frac{16r_s k_F}{\pi^2 q} F(q) I(q) \ln \left| \frac{q + 2k_F}{q - 2k_F} \right|}. \quad (15)$$

where $\rho(\varepsilon_F) = 2m^*/\pi k_F$ is the density of states at the Fermi energy in one dimensional electron gas. Note that the Pauli spin susceptibility is $\chi_{Pauli} = \mu_B^2 \rho(\varepsilon_F)$ [17].

3 Results and Discussion

The results presented in this section are obtained by solving Eqs. (4), (7) and (8) self-consistently. In Fig. 1, the magnetic structure factor $\tilde{S}(q)$ is presented for different r_s values for a wire of effective radius $b = 2a_B^*$. The appearance of a peak at $q = 2k_F$ as the density decreases has also been reported in earlier studies[12]. It gets progressively difficult to achieve convergence in the self-consistent calculation for $r_s > 1.8$. An instability sets in at this value of r_s , as also observed in earlier STLS studies[12],[13]. This unfortunately means that we are unable to study different possible phases of the 1D electron gas as one varies the density or equivalently the r_s parameter.

The magnetic structure factor $\tilde{S}(q)$ obtained using different approaches is shown in Fig. 2. It seems that the Hubbard approximation has the most pronounced peak at shown values of r_s and the wire radius b . The sharpness of the SSTL peak comes out to be the least.

In contrast to $\tilde{S}(q)$, the static structure factor $S(q)$ is easier to obtain even for larger values of r_s , as observed also in earlier work[16]. The $S(q)$ for $r_s = 2$, and different values of the effective wire radii are shown in Fig. 3.

The static local field corrections arising from the short range Coulomb correlation and exchange-correlation effects for the density and spin-density responses are shown in Figs. 4 and 5, respectively.

The spin dependent pair correlation functions $g_{\uparrow\uparrow}(r)$ and $g_{\uparrow\downarrow}(r)$ are shown in Figs. 6 and 7, respectively, for different r_s values. It is seen that $g_{\uparrow\uparrow}(r)$ has very weak r_s dependence.

The spin symmetric and anti symmetric effective potentials $\psi_{\uparrow\uparrow}(q)$ and $\psi_{\uparrow\downarrow}(q)$ in units of $V(q)$ are shown in Figs. 8 and 9. They are also compared with the STLS results. The effective potentials have rather similar behaviour in both cases.

The static density susceptibility function is compared with STLS result in Fig. 10. The static spin-density susceptibility, on the other hand, is compared with STLS and HA results in Fig. 11. It is seen that the results in all three approaches are qualitatively and quantitatively similar. The peak at $q = 2k_F$ is less pronounced in the SSTL approach which seems to be its dominant character.

Collective excitations in the one dimensional electron gas can be studied as the poles of the density and spin-density response functions $\chi^{d,s}(q, \omega)$. The dispersion of the paramagnon peak, $\omega_p(q)$ is shown in Fig. 12 for $r_s = 1.5$. For small q , $\omega_p(q)$ shows a linear behaviour, as also observed before in STLS work[12].

In summary, we have studied the spin correlations in a one dimensional electron gas, and have shown that the SSTL approach is capable of giving results qualitatively similar to those obtained by using the STLS approach. This is, of course, not enough to establish the performance of the SSTL approach in 1D. The question of compressibility inconsistency should be settled before one considers the SSTL approach as a viable alternative to other approaches.

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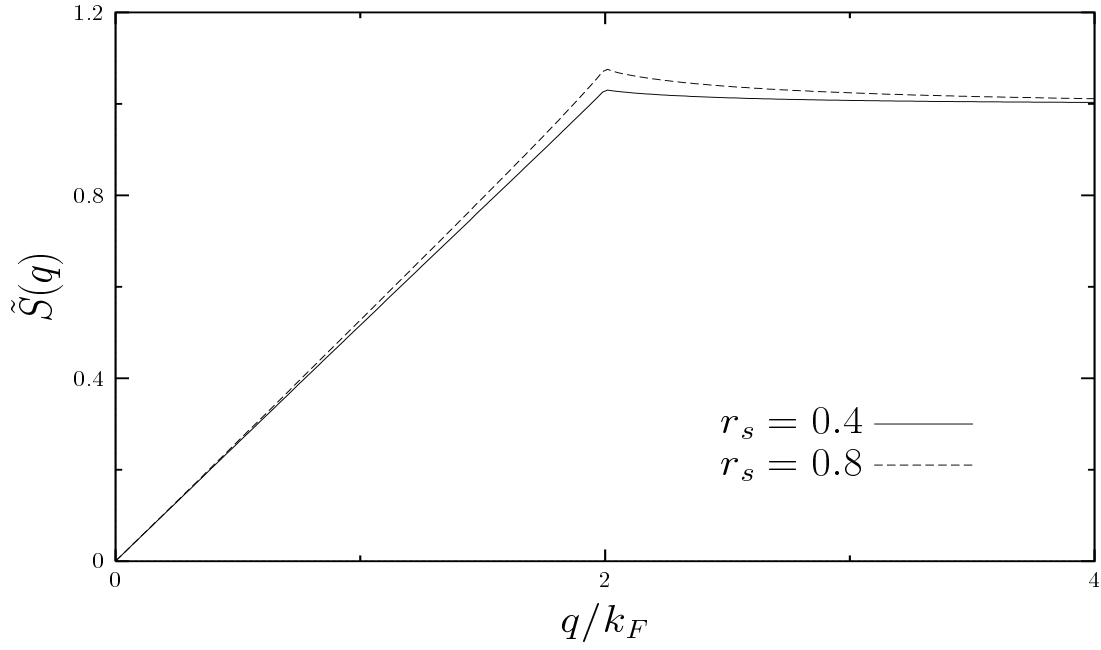


Figure 1: The magnetic structure factor $\tilde{S}(q)$ for different r_s values at wire radius $b = 2a_B^*$ in the SSTL approximation.

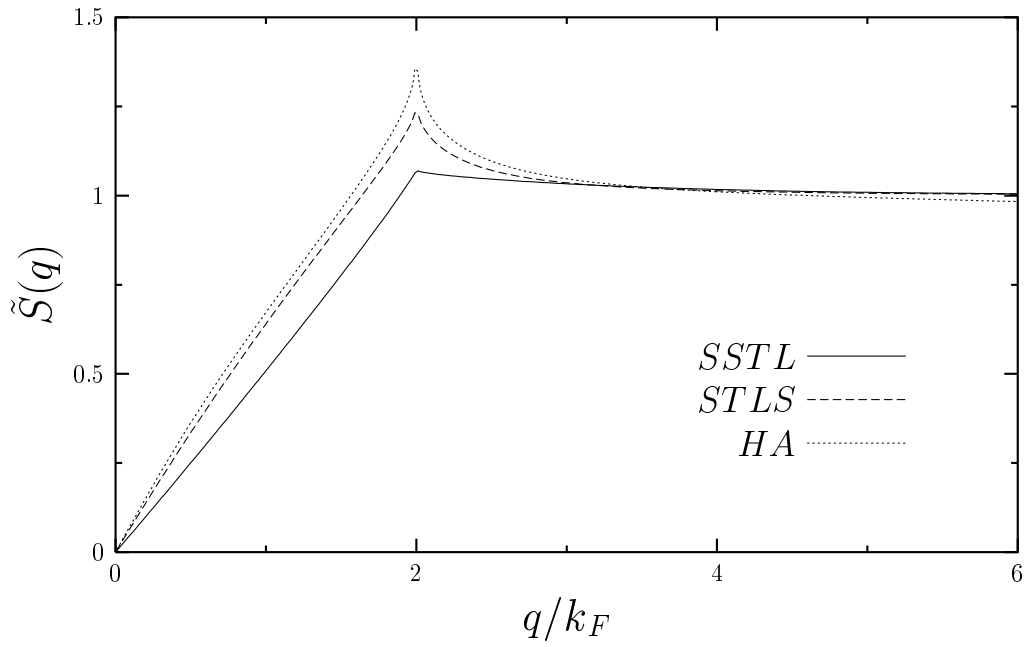


Figure 2: The magnetic structure factor $\tilde{S}(q)$ at $r_s = 1$ and $b = 2a_B^*$ in different approximations.

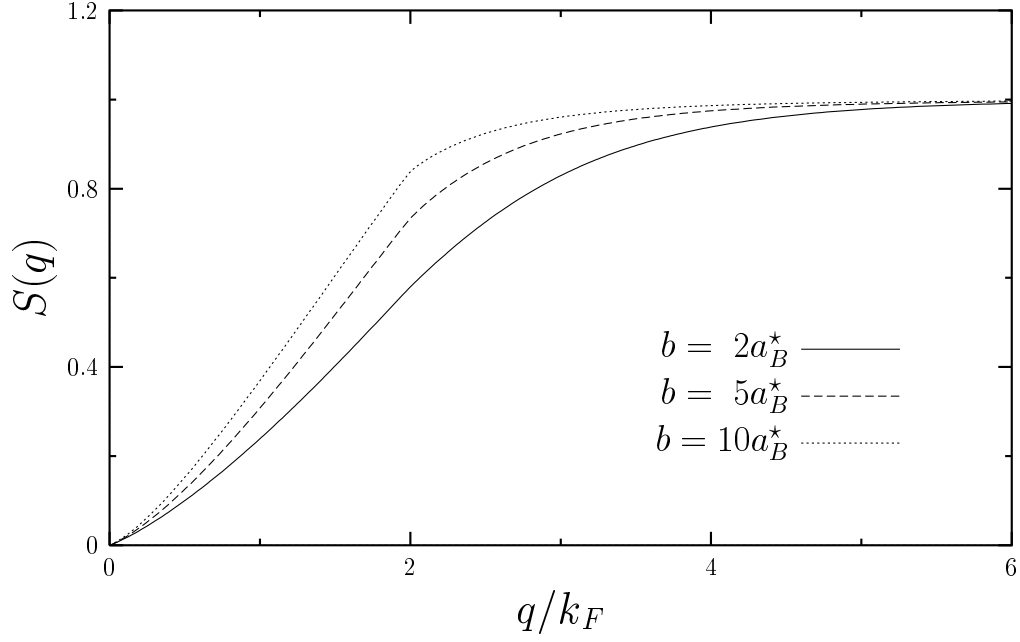


Figure 3: The static structure factor $S(q)$ at $r_s = 2$ for different wire radii in the SSTL approximation.

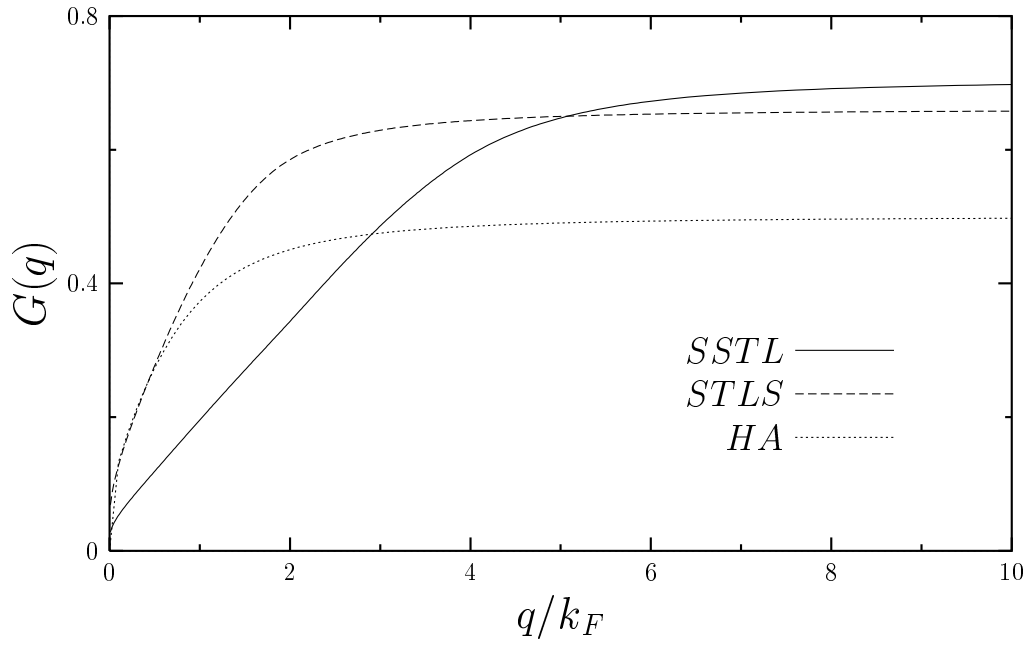


Figure 4: The density local field correction $G(q)$ in different approximations for $r_s = 1$ and $b = 2a_B^*$.

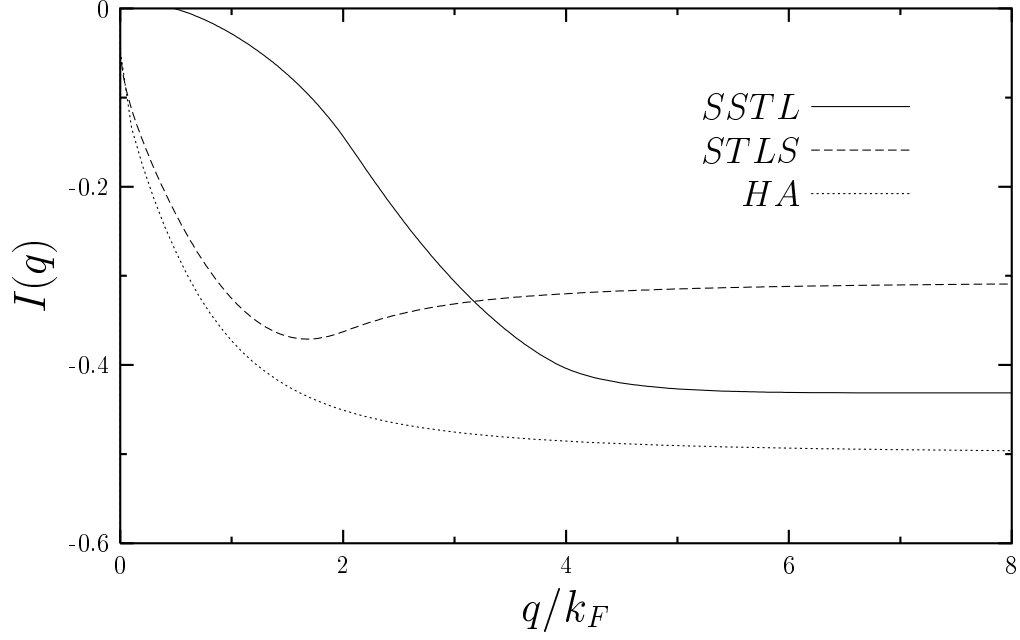


Figure 5: The spin-density local field correction $I(q)$ in different approximations for $r_s = 1$ and $b = 2a_B^*$.

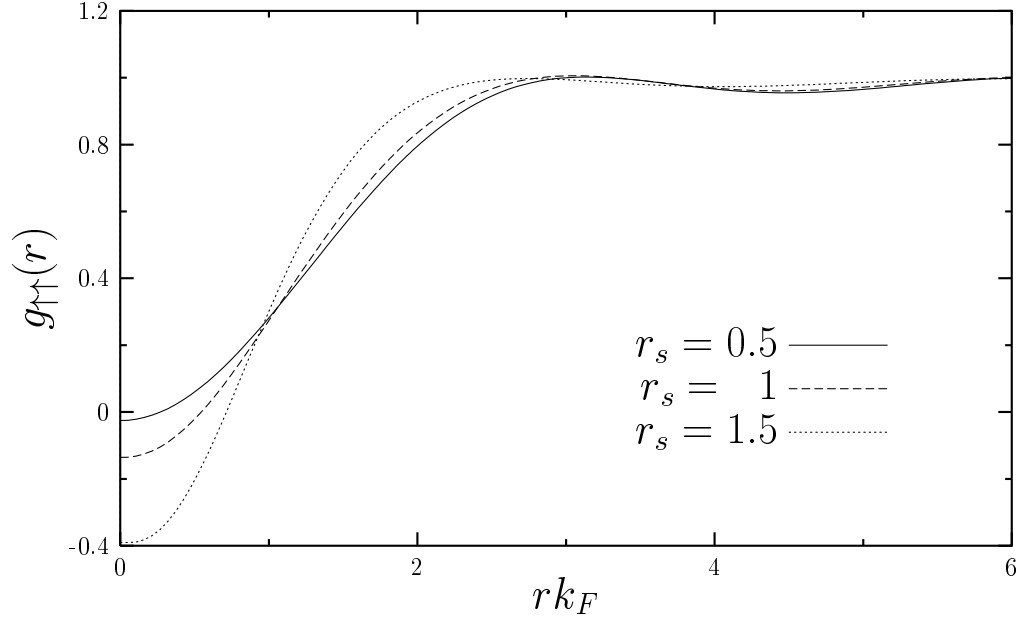


Figure 6: The spin dependent pair correlation function $g_{\uparrow\uparrow}(r)$ for $b = 2a_B^*$ and several r_s values in the SSTL approximation.

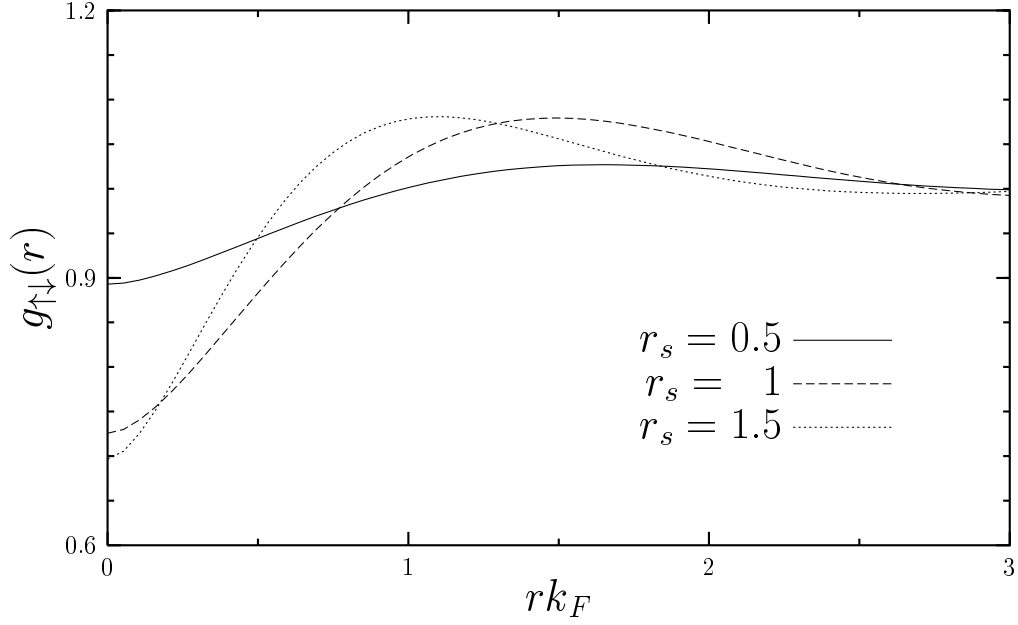


Figure 7: The spin dependent pair correlation function $g_{\uparrow\downarrow}(r)$ for $b = 2a_B^*$ and several r_s values in the SSTL approximation.

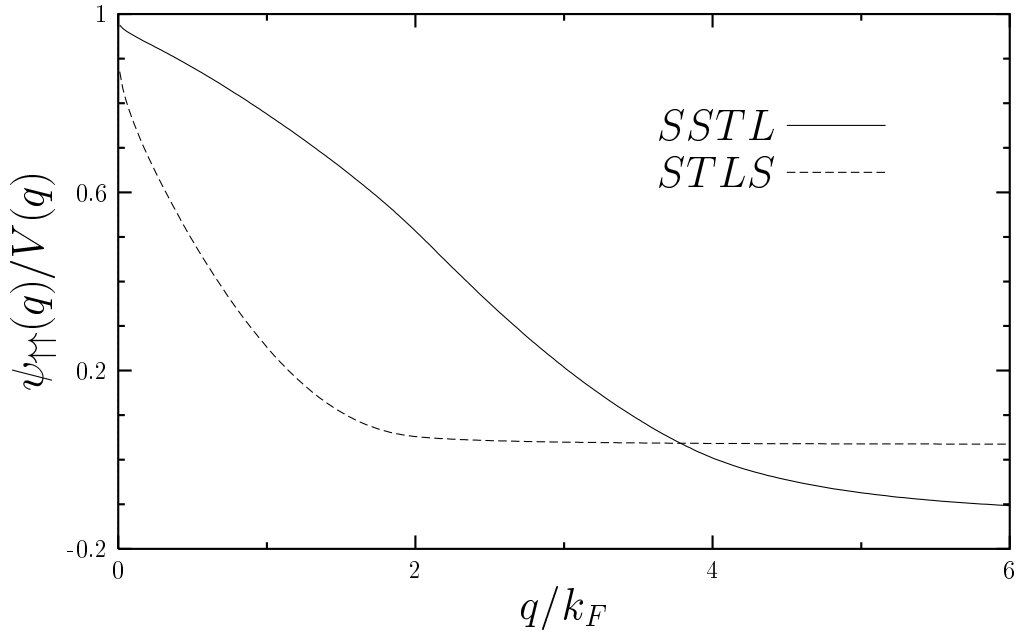


Figure 8: The spin dependent effective potential $\psi_{\uparrow\uparrow}(q)$ in units of $V(q)$ for $r_s = 1$ and $b = 2a_B^*$ in the SSTL and STLS approximations.

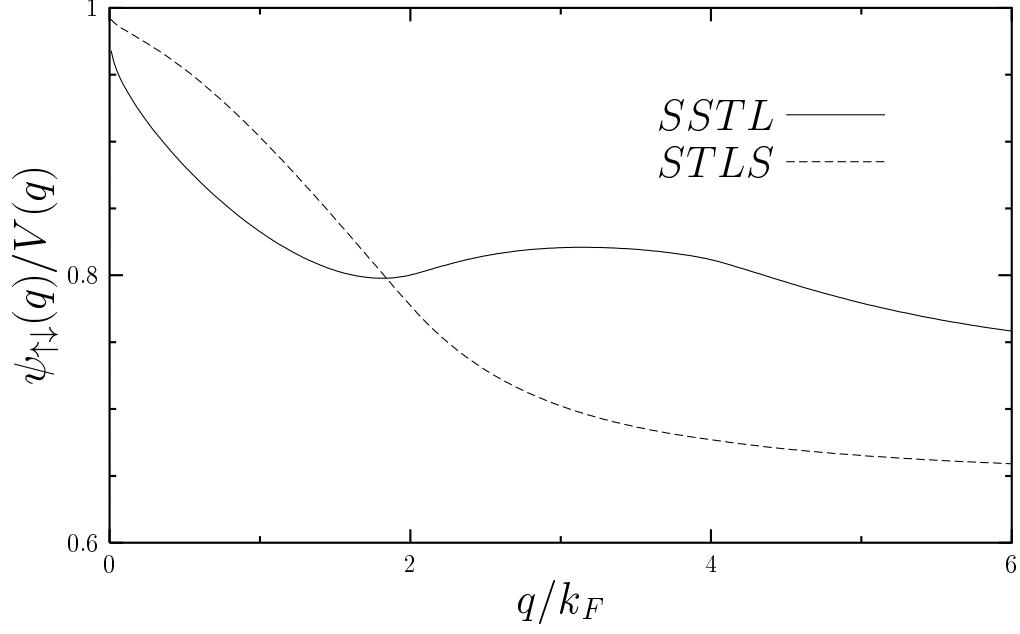


Figure 9: The spin dependent effective potential $\psi_{\uparrow\downarrow}(q)$ in units of $V(q)$ for $r_s = 1$ and $b = 2a_B^*$ in the SSTL and STLS approximations.

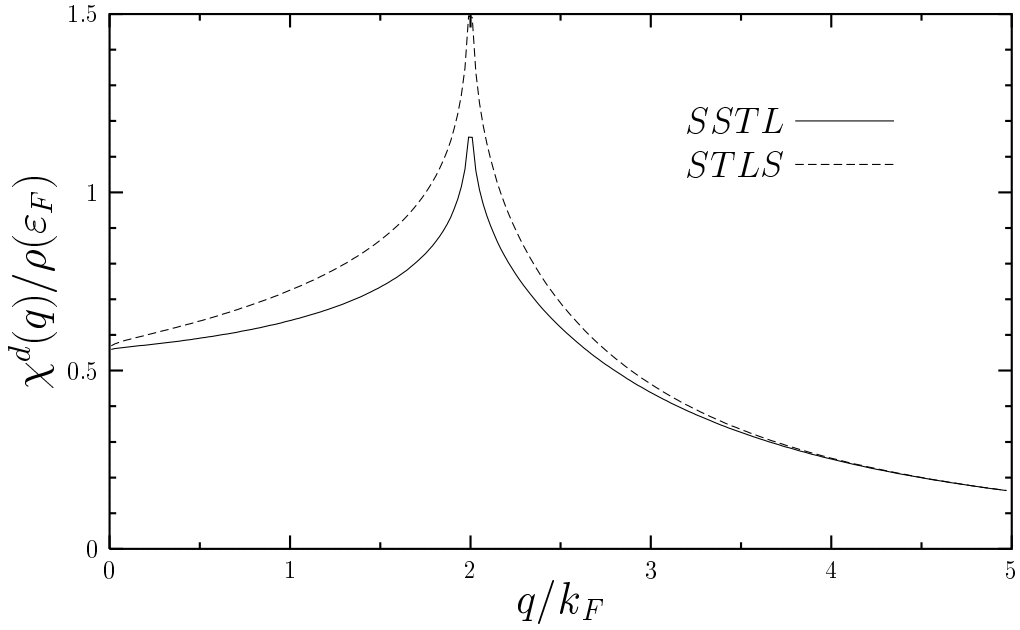


Figure 10: The static density response $\chi^d(q)$ in units of $\rho(\varepsilon_F)$ for $r_s = 1$ and $b = 2a_B^*$ in SSTL and STLS approximations.

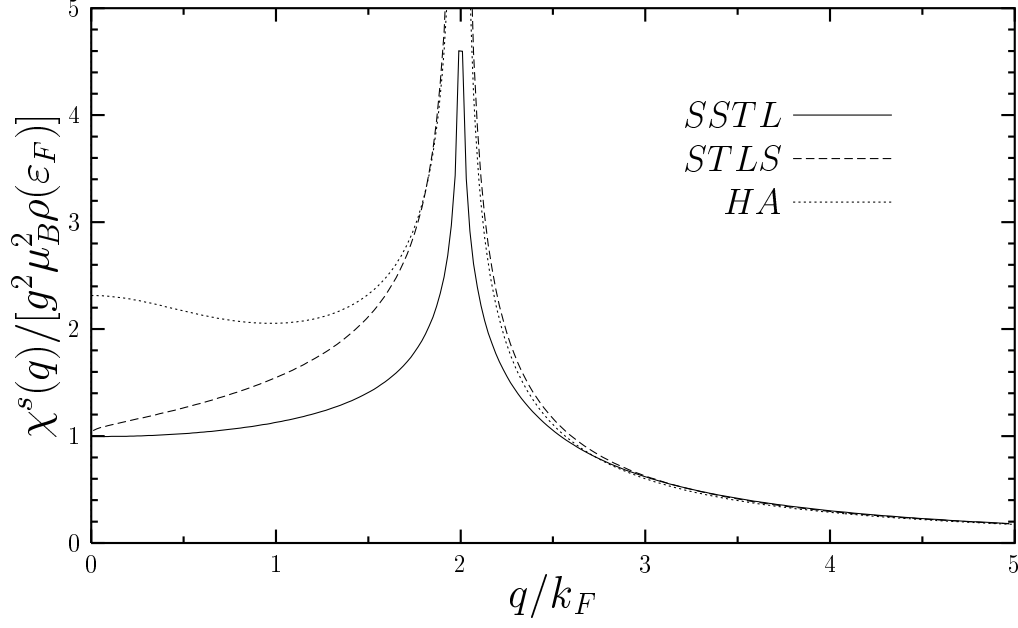


Figure 11: The static spin response $\chi^s(q)$ in units of $g^2 \mu_B^2 \rho(\varepsilon_F)$ for $r_s = 1$ and $b = 2a_B^*$ in different approximations.

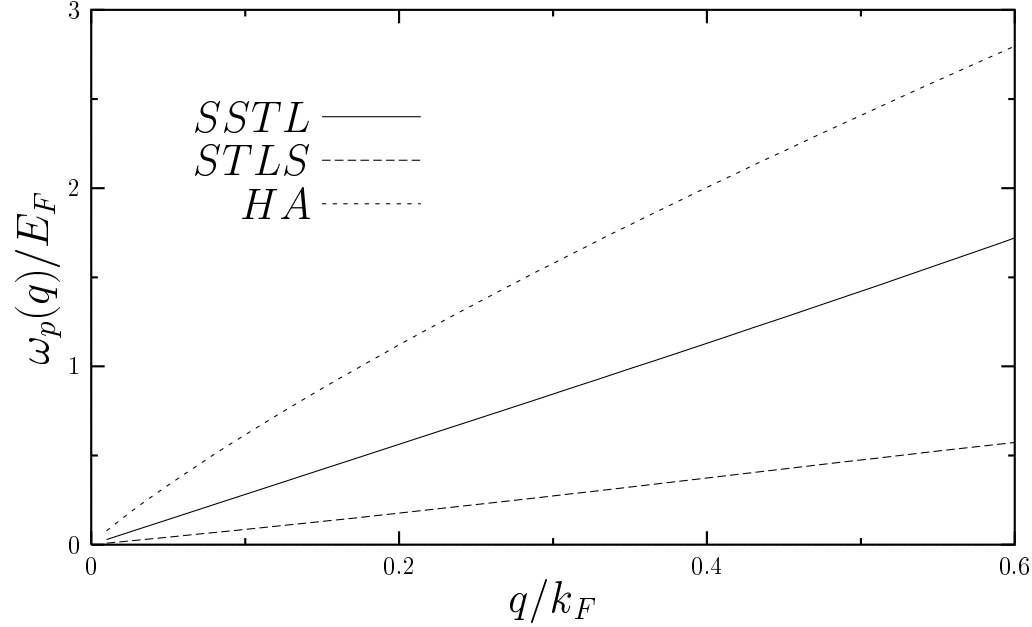


Figure 12: The dispersion of the paramagnon peak $\omega_p(q)$ in units of E_F for $r_s = 1.5$ and $b = 2a_B^*$ in different approximations.